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Coherent transport: Landauer-Büttiker method

Quantum junctions • Landauer formula • Multi-channel scattering and transport
Multi-terminal systems • Problems

The Landauer-Büttiker (LB) method (also known as the scattering method) establishes the relation between the wave functions (scattering amplitudes) of electrons in a nanojunction and the conducting properties of this junction. The LB method can be applied to find the current through a noninteracting junction or through a junction with effectively noninteracting quasiparticles, for example if the mean-field description is valid and the inelastic scattering is not essential. Such type of an electron transport is called *coherent*, because there is no phase-breaking and quantum interference is preserved during the electron motion across the system. Actually, the LB method is now routinely applied to basic transport calculations through nanostructures and single molecules. Besides, it is directly applicable in many semiconductor quantum dot systems with weak electron-electron interaction. Due to simplicity and generality of the LB method, it is now widely accepted and is in the base of our understanding of the coherent transport.

In this chapter we consider the foundations and some applications of the LB method, related directly to the problems of quantum transport at nanoscale. At the beginning (section 1.1) we discuss a basic quantum junction model and introduce necessary results from the quantum scattering theory. Then we obtain the Landauer formula in the single-channel (and independent-channel) case and discuss its physical sense (section 1.2). In section 1.3 the general multi-channel formalism is discussed, and in section 1.4 the multi-terminal case is considered.

Some additional topics, such as noise, thermal transport, hybrid systems with superconducting and magnetic electrodes, are briefly discussed in section **??**. Many other extensions of the method are beyond our consideration. One can mention the LB method in combination with random matrix theory, localization theory, the attempts to introduce the analogous scattering description for interacting and dissipative systems. However, in spite of such popularity of the LB method, one should remember, that in its canonical form it is applicable only for noninteracting systems.

1.1 Quantum junctions

1.1.1 Electrodes, leads, scatterer

As we already discussed in the Introduction, a nanojunction consists of three parts: left and right large equilibrium electrodes and central nanoscale region. In this chapter we neglect possible discrete nature of the central region and consider the nanojunction as a continuous medium. Moreover, we assume, that transport is completely coherent between the electrodes. It means that we neglect all inelastic effects inside the central region. The electrodes, however, are equilibrium and incoherent by definition, because the equilibrium state is established as a result of energy relaxation due to inelastic scattering. If an electron comes from the central region into the electrode, it is thermalized and any phase information is lost. On the other hand, electrons, which enter to the central region from the electrodes with random phases, keep the phase information until they return back to the electrodes, but their distribution function in the central part is determined by the boundary conditions and is nonequilibrium at finite voltage. For further consideration it is convenient to divide the central region into quantum leads and scattering region, or scatterer (Fig. 1.1).

Transport through a coherent region can be described by a wave function. The leads serve as quantum waveguides for electrons. They connect the electrodes with the scattering region and are assumed to have a well defined mode structure: incoming (from the left or right, $s = L, R$, electrode to the scatterer) modes $\psi_{s+}(\mathbf{r})$ and outgoing modes $\psi_{s-}(\mathbf{r})$ can be defined. In the simplest case the leads are noninteracting, but nonequilibrium at finite biased voltage. The scattering region can be as simple as one tunneling barrier or impurity, or as complex as an interacting nonequilibrium molecule. In the continuous case the scatterer is described by some potential $U(\mathbf{r})$, it results from impurity scattering or external potential.

Note, that the boundaries between electrodes, leads and scatterer are to a certain extent arbitrary. It is important only to take all conduction modes (transport channels) into account.
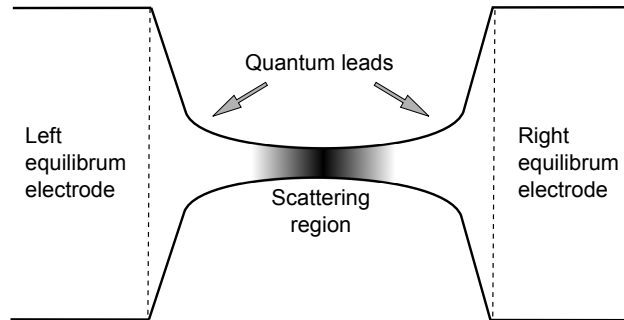

Fig. 1.1. Schematic picture of a quantum junction: the scattering region is connected to the electrodes trough the quantum leads.

1.1.2 Transport channels

Let us introduce the important concept of transport channels. To start, we simplify the problem, assuming that the motion of electrons is effectively one-dimensional. For this purpose we factorize the wave function with some energy E in the following form:

$$\Psi_E(\mathbf{r}) = \sum_n \phi_n(x,y,z)\,\psi_{nE}(z),$$ (1.1)

where z axis denote the direction of electron motion, $\phi_n(x,y,z)$ describes the transverse structure, n is called *mode* or *channel* index. At the first glance, we only complicated the problem, because instead of one unknown function we got many. But the trick is that the solution for $\phi_n(x,y,z)$ can be easily obtained in many cases and we should solve only the equation for $\psi_{nE}(z)$. For example, in 3D layered systems a corresponding solution is

$$\Psi_E(\mathbf{r}) = \sum_{\mathbf{k}} e^{i(k_x x + k_y y)}\,\psi_{\mathbf{k}E}(z),$$ (1.2)

where $\mathbf{k}$ is the wave vector parallel to the layers. Initial 3D problem is reduced in this case to a 1D problem for the function $\psi_{kE}(z)$. Similar situation takes place in the effectively 1D or 2D spatially quantized systems (electronic waveguides), where $\phi_{nE}(x,y,z)$ describes different transverse modes at different n.

To understand better, how transport channels are formed, let us consider two examples (Fig. 1.2): a constant cross-section waveguide and an adiabatic waveguide (quantum point contact). Such quantum waveguides for electrons can be three-dimensional or formed from 2D electron gas, in the last case the motion in y direction is quantized and y coordinate is absent in the equations below.

The wave functions are calculated from the Schrödinger equation

$$\left\{ -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) + U(x,y,z) \right\} \Psi_E(x,y,z) = E\Psi_E(x,y,z),$$ (1.3)

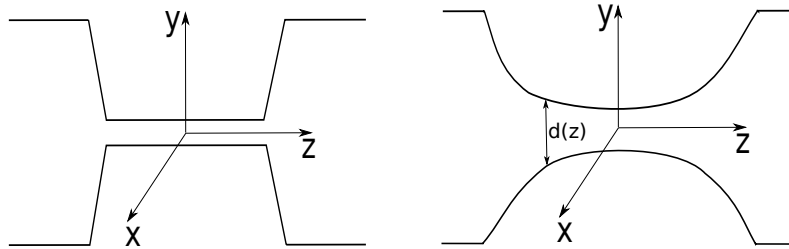where $U(x,y,z)$ is the external potential, defining the geometry of the junction.

Fig. 1.2. Waveguides of constant cross-section (left) and adiabatic.

For waveguides with constant cross-section $U(x,y)$ is z-independent, and the solution can be presented in the form (1.1) exactly as

$$\Psi_E(\mathbf{r}) = \sum_n \phi_n(x,y)e^{ik_nz}, \qquad (1.4)$$

with the wave vectors $\hbar k_n = \pm\sqrt{2m(E-E_n)}$, E_n are the transverse energy eigenvalues. From this expression it is clear, that the number of propagating modes (called *open* channels) at given energy E equals to the number of transverse modes with $E_n < E$:

$$N_{ch}(E) = \sum_n \theta(E-E_n). \qquad (1.5)$$

At $E_n > E$ the wave number is imaginary and this mode can exist only at the end of the waveguide, these channels are called *closed*. It is important that N_{ch} is a function of energy and can be changed if the Fermi energy or the gate voltage are changed.

Adiabatic junction

Now we consider a waveguide with the variable cross-section. In the adiabatic approximation the spatial variation in the z-direction is much slower than in transverse directions. Thus, the second derivative with respect to z is small and it is reasonable to consider the Scrödinger equation for the transverse eigenfunctions $\phi_n(x,y)$ with z as a parameter

$$\left\{-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}\right)+U(x,y,z)\right\}\phi_n(x,y,z) = E_n(z)\phi_n(x,y,z), \qquad (1.6)$$

$E_n(z)$ is the (position-dependent) energy eigenvalue. If we substitute the Ansatz (1.1) with these eigenfunctions into (1.3) and neglect again the derivatives of $\phi_n(x,y,z)$ in the z-direction, we get the 1D equation for the function $\psi_{nE}(z)$:

$$\left\{-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial z^2}+E_n(z)\right\}\psi_{nE}(z) = E\psi_{nE}(z), \qquad (1.7)$$

where the energy $E_n(z)$ plays the role of an effective potential.

Consider a simple example, namely a 2D junction with the hard-wall potential. Assume, that the size of the waveguide in x-direction is $d(z)$. The transverse solution (at fixed z) is

$$\phi_n(x,z) = \sqrt{\frac{2}{d(z)}}\sin\left(\frac{2\pi n(x+d(z)/2)}{d(z)}\right), \qquad (1.8)$$

and corresponding energy eigenvalue, e.g. the effective potential for z motion is

$$E_n(z) = \frac{\hbar^2\pi^2 n^2}{2md^2(z)}. \qquad (1.9)$$

If we plot now this energy as a function of z (Fig. 1.3), we can determine, which channels are open at given energy E. It will be all channels with the maximum $E_n(z)$
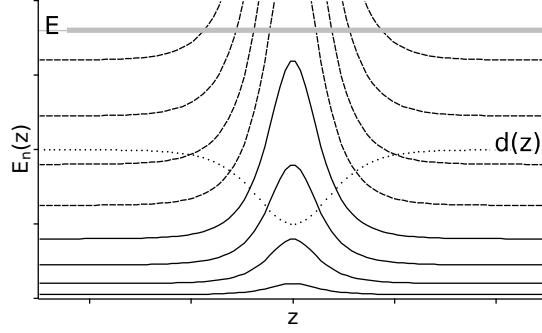
Fig. 1.3. Effective potential energy $E_n(z)$. The open transport channels are shown by solid lines, closed one – by dashed lines. The dotted line shows $d(z)$.

being smaller than E. Note, that if the maximum $E_n(z)$ is close to the energy, the channel is only partially open, because both scattering and transmission are possible with some probabilities. For adiabatic junctions, however, this energy interval is very small, and all channels can be considered to be open or closed.

The condition of adiabaticity in two dimensional junctions can be written as $\partial d(z)/\partial z \ll \lambda_F/d(z)$. On the other hand, the position-dependent number of open channels is $N(z) = k_F d(z)/\pi$ and one gets

$$\frac{\partial d(z)}{\partial z} \ll \frac{1}{N(z)}. \tag{1.10}$$

This condition shows, that it is much easier to obtain the adiabatic transport for narrow junctions with small number of channels.

In the above considered examples the channels are independent, there are no transitions between different modes. This type of transport can be named *mode-conserving*. Below in this and next sections we consider only single channel and independent channels. More general situation with inter-mode scattering will be consider in the section 1.3.

1.1.3 Reflection and transmission

As one can see, the main formal problem to be solved in the Landauer theory is the single-particle scattering problem. The conductance is determined then from the elements of the transmission matrix. For this reason, the LB method is called also a scattering method. In the following sections we introduce the basic notions of the quantum scattering theory, and formulate them in the form convenient for further calculations.

Now consider a one-dimensional potential (schematic in Fig. 1.4) which is constant far from the scattering region: $U(z \to -\infty) = 0$, $U(z \to \infty) = U_0$. Thus, the wave function in the state with the energy E_z (the full energy $E = E_n + E_z$ is assumed to be the sum of E_z and the transverse energy E_n), and incident from the left, is
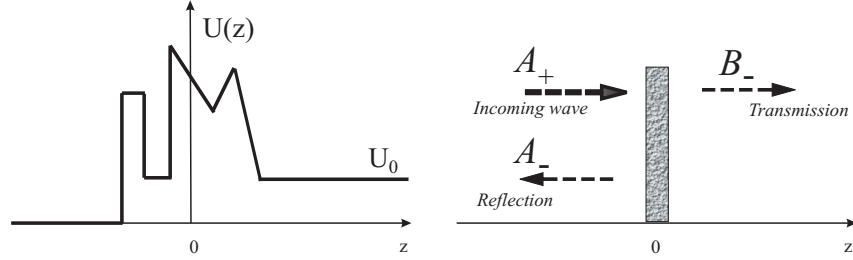
Fig. 1.4. One-dimensional potential. Reflection and transmission.

$$\psi(z \to -\infty) = A_+ e^{ikz} + A_- e^{-ikz}, \tag{1.11}$$

$$\psi(z \to +\infty) = B_- e^{ik'z}, \tag{1.12}$$

where A_+ is the incoming and A_-, B_- are the outgoing waves (Fig. 1.4). Wave vectors k and k' are defined as

$$k = \frac{\sqrt{2mE_z}}{\hbar}, \tag{1.13}$$

$$k' = \frac{\sqrt{2m(E_z - U_0)}}{\hbar}. \tag{1.14}$$

To determine the transmission and reflection probabilities, one should use the conservation of probability flux density ("current")

$$\mathbf{f} = \frac{i\hbar}{2m} \left[\psi(\mathbf{r})\nabla \psi^*(\mathbf{r}) - \psi^*(\mathbf{r})\nabla \psi(\mathbf{r}) \right]. \tag{1.15}$$

From the Schrödinger equation the conservation law follows:

$$\frac{\partial |\psi(\mathbf{r},t)|^2}{\partial t} + \mathrm{div}\mathbf{f} = 0, \tag{1.16}$$

which in the stationary case is simply

$$\mathrm{div}\mathbf{f} = 0. \tag{1.17}$$

For the plane wave Ae^{ikz} the probability flux density ("current") is reduced to

$$f = \frac{\hbar k}{m} |A|^2 = v|A|^2, \tag{1.18}$$

where we introduced the velocity $v = \hbar k/m$.

Now we are ready to define the *transmission coefficient* as the ratio of the transmitted to incident probability flux

$$T(E_z) = \frac{f_{tran}}{f_{inc}} = \frac{v_\infty |B_-|^2}{v_{-\infty} |A_+|^2} = \frac{k'}{k} \frac{|B_-|^2}{|A_+|^2}, \tag{1.19}$$
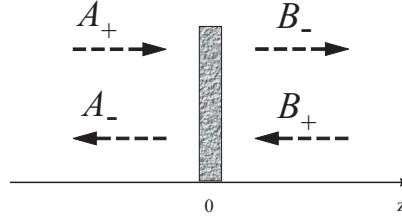
Fig. 1.5. Single barrier. General scattering problem.

and the *reflection coefficient* as the ratio of the reflected to the incident probability flux

$$R(E_z) = \frac{f_{ref}}{f_{inc}} = \frac{|A_-|^2}{|A_+|^2}. \tag{1.20}$$

From the probability flux conservation it follows that

$$T(E_z) + R(E_z) = 1. \tag{1.21}$$

Note, that if we consider the incident wave *from the right side* of the barrier, the transmission coefficient is the same at the same energy

$$T_{R \to L}(E_z) = T_{L \to R}(E_z). \tag{1.22}$$

1.1.4 Scattering and transfer matrices

Now we consider the general scattering (or transmission) problem, assuming that there are incoming modes from the left and from the right sides of the barrier (Fig. 1.5).

δ -potential

We start from the δ-potential (some other barriers are considered in Problems 1.2-4)

$$U(z) = \alpha \delta(z). \tag{1.23}$$

The solution is given by

$$\psi(z) = \begin{cases} A_+ e^{ikz} + A_- e^{-ikz}, \ z < 0, \\ B_- e^{ikz} + B_+ e^{-ikz}, \ z > 0, \end{cases} \tag{1.24}$$

where A_+, B_+ are incoming and A_-, B_- are outgoing waves, $k = \dfrac{\sqrt{2mE_z}}{\hbar}$. The boundary conditions at the δ-potential are

$$\psi(0-) = \psi(0+), \tag{1.25}$$

$$\psi'(0+) - \psi'(0-) = \frac{2m\alpha}{\hbar^2} \psi(0). \tag{1.26}$$

We can represent this boundary condition using *the transfer matrix* $\hat{M}$: $\left(K = \dfrac{\hbar^2 k}{m\alpha} \right)$

$$\begin{pmatrix} A_+ \\ A_- \end{pmatrix} = \hat{M} \begin{pmatrix} B_- \\ B_+ \end{pmatrix} = \begin{pmatrix} 1+\frac{i}{K} & \frac{i}{K} \\ -\frac{i}{K} & 1-\frac{i}{K} \end{pmatrix} \begin{pmatrix} B_- \\ B_+ \end{pmatrix}, \tag{1.27}$$

or, alternatively, *the scattering matrix* $\hat{S}$:

$$\begin{pmatrix} A_- \\ B_- \end{pmatrix} = \hat{S} \begin{pmatrix} A_+ \\ B_+ \end{pmatrix} = \begin{pmatrix} \frac{1}{iK-1} & \frac{iK}{iK-1} \\ \frac{iK}{iK-1} & \frac{1}{iK-1} \end{pmatrix} \begin{pmatrix} A_+ \\ B_+ \end{pmatrix}. \tag{1.28}$$

The transfer matrix relates the states from two sides of the barrier, while the scattering matrix relates the amplitudes of outgoing waves to the amplitudes of incoming waves.

To find the transmission and reflection coefficients we set now $B_+ = 0$, then

$$T(E) = \left[\frac{\upsilon_L}{\upsilon_R} \right] \frac{|B_-|^2}{|A_+|^2} = \left[\frac{\upsilon_L}{\upsilon_R} \right] \frac{1}{|M_{11}|^2} = \left[\frac{\upsilon_L}{\upsilon_R} \right] |S_{21}|^2 = \frac{K^2}{1+K^2}, \tag{1.29}$$

$$R(E) = \frac{|A_-|^2}{|A_+|^2} = \frac{|M_{21}|^2}{|M_{11}|^2} = |S_{11}|^2 = \frac{1}{1+K^2}, \tag{1.30}$$

$$T + R = 1.$$

We use here the square brackets to show the terms, which appear for the junctions with different left and right velocities υ, see the Problems 1.3, 1.4 for detailed calculations.

The descriptions in terms of scattering or transfer matrices are completely equivalent and the choice is only dependent on the convenience and the problem to be solved. Typically, in the end of a calculation the $\hat{S}$-matrix should be obtained, because it determines the conductivity by the Landauer formula. But to calculate the scattering by the complex system, the $\hat{M}$-matrix can be convenient, as we shall see in the next section.

Some general properties of $\hat{S}$ and $\hat{M}$ matrices

In general case (asymmetric junction, magnetic field, etc.) the scattering matrix is usually represented as

$$\hat{S} = \begin{pmatrix} r & t' \\ t & r' \end{pmatrix}. \tag{1.31}$$

The reflection and transmission coefficients *from left to right* are

$$T_{L \to R}(E) = \frac{\upsilon_L}{\upsilon_R} |t|^2; \quad R_{L \to R}(E) = |r|^2, \tag{1.32}$$

and *from right to left*

$$T_{R\to L}(E) = \frac{v_R}{v_L}|t'|^2; \quad R_{R\to L}(E) = |r'|^2. \tag{1.33}$$

The transfer matrix can be written explicitly in terms of transmission and reflection amplitudes r, r', t, t' as

$$\hat{M} = \begin{pmatrix} \dfrac{1}{t} & -\dfrac{r'}{t} \\ \dfrac{r}{t} & \dfrac{tt'-rr'}{t} \end{pmatrix}, \tag{1.34}$$

as well the scattering matrix in terms of the elements of $\hat{M}$ as

$$\hat{S} = \begin{pmatrix} \dfrac{M_{21}}{M_{11}} & \dfrac{M_{11}M_{22}-M_{12}M_{21}}{M_{11}} \\ \dfrac{1}{M_{11}} & -\dfrac{M_{12}}{M_{11}} \end{pmatrix}. \tag{1.35}$$

For symmetric leads ($v_L = v_R$) the S-matrix is unitary

$$\hat{S}\hat{S}^\dagger = \hat{I}, \tag{1.36}$$

so that

$$|r|^2 + |t|^2 = 1, \quad |r'|^2 + |t'|^2 = 1, \quad r^*t' + t^*r' = 0. \tag{1.37}$$

For asymmetric leads ($v_L \neq v_R$), however, the S-matrix (as we defined it up to now) is obviously not unitary, because of additional velocity factors in the expression (1.19) for the transmission coefficient. If one needs to have the unitary matrix, it is possible to redefine it as

$$S'_{nm} = \sqrt{\frac{v_n}{v_m}} S_{nm}. \tag{1.38}$$

Or, equivalently, redefine the amplitudes of plane waves as $Ae^{ikz} = (A'/\sqrt{v})e^{ikz}$, and the flux density

$$f = \frac{\hbar k}{m}|A|^2 = v|A|^2 = |A'|^2. \tag{1.39}$$

Below we always assume that the S-matrix is unitary, and the reflection and transmission coefficients acquire the simple form

$$T_{L\to R}(E) = |t|^2; \quad R_{L\to R}(E) = |r|^2,$$
$$T_{R\to L}(E) = |t'|^2; \quad R_{R\to L}(E) = |r'|^2. \tag{1.40}$$

In the time-reversal case (no magnetic field) the product of the S-matrix with its complex conjugate is the unity matrix

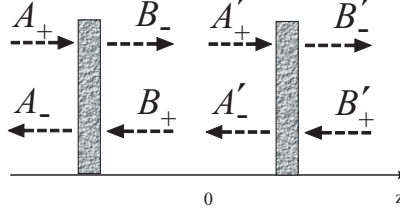$$\hat{S}\hat{S}^* = \hat{I}, \tag{1.41}$$

from which follows

Fig. 1.6. Double barrier.

$$|r'|^2 = |r|^2, \quad |r|^2 + t^* t' = 1, \quad |t'|^2 = |t|^2, \tag{1.42}$$

and

$$R_{L \to R}(E) = R_{R \to L}(E); \quad T_{L \to R}(E) = T_{R \to L}(E). \tag{1.43}$$

Note, finally, that an unitary matrix in the time reversal case is symmetric, and $|r| = |r'|$, so that the S-matrix can be represented in the form

$$\hat{S} = \begin{pmatrix} r & t \\ t & re^{i\theta} \end{pmatrix}. \tag{1.44}$$

A series of scatterers: transfer matrix method

If one has a series of scatterers, the calculation of the resulting transfer matrix can be simplified by the use of the transfer matrices of single scatteres. Consider two sequential barriers with transfer matrices $\hat{M}$ and $\hat{M}'$ (Fig. 1.6), so that

$$\begin{pmatrix} A_+ \\ A_- \end{pmatrix} = \hat{M} \begin{pmatrix} B_- \\ B_+ \end{pmatrix}, \quad \begin{pmatrix} A'_+ \\ A'_- \end{pmatrix} = \hat{M}' \begin{pmatrix} B'_- \\ B'_+ \end{pmatrix}. \tag{1.45}$$

In the case when both $\hat{M}$ and $\hat{M}'$ are calculated independently, assuming that the barrier is placed at $z = 0$, the outgoing coefficients B and incoming coefficients A' are related by the propagation transfer matrix $\hat{M}_L$

$$\begin{pmatrix} B_- \\ B_+ \end{pmatrix} = \hat{M}_L \begin{pmatrix} A'_+ \\ A'_- \end{pmatrix} = \begin{pmatrix} e^{-ikL} & 0 \\ 0 & e^{ikL} \end{pmatrix} \begin{pmatrix} A'_+ \\ A'_- \end{pmatrix}. \tag{1.46}$$

To show that in the most simple way, note that $B_- e^{ikz}$ and $A'_+ e^{ikz}$ describe the same plane wave in two different points $z = 0$ and $z = L$, the phase difference is obviously kL.

Finally we can write

$$\begin{pmatrix} A_+ \\ A_- \end{pmatrix} = \hat{M}_T \begin{pmatrix} B'_- \\ B'_+ \end{pmatrix} = \hat{M}\hat{M}_L\hat{M}' \begin{pmatrix} B'_- \\ B'_+ \end{pmatrix}. \tag{1.47}$$

Thus, the transfer matrix for a sequence of barriers can be defined as the product of the particular transfer matrices of the barriers and the propagating transfer matrices

$$\hat{M}_T = \hat{M}_1 \hat{M}^L_{1,2} \hat{M}_2 ... \hat{M}_n \hat{M}^L_{n,n+1} \mathbf{M_{n+1}} ... \hat{M}_{N-1} \hat{M}^L_{N-1,N} \hat{M}_N. \tag{1.48}$$

Breit-Wigner formula

As an example, we can calculate the transmission coefficient for the double-barrier system. We need only M_{T11} because it determines T (see (1.29)) and $R = 1 - T$. The transfer matrix $\hat{M}_T$ for a two-barrier structure is

$$\hat{M}_T = \hat{M}\hat{M}_L\hat{M}' = \begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix} \begin{pmatrix} e^{-ikL} & 0 \\ 0 & e^{ikL} \end{pmatrix} \begin{pmatrix} M'_{11} & M'_{12} \\ M'_{21} & M'_{22} \end{pmatrix}. \tag{1.49}$$

$$M_{T11} = M_{11}M'_{11}e^{-ikL} + M_{12}M'_{21}e^{ikL} \tag{1.50}$$

In the case of two identical barriers, for transmission coefficient we find

$$T(E) = \frac{T_1^2}{T_1^2 + 4R_1 \cos^2(kL - \theta)}, \tag{1.51}$$

where θ is the phase of the complex M_{11}. T_1 and R_1 are transmission and reflection coefficients of the single barrier.

From this general expression one can see the important property of two-barrier structures: there are transmission resonances, at some specific energies E_n the transmission coefficient is large ($T(E_n) = 1$ in symmetric structures), while between resonances it can be small.

When the barriers are δ-functions $M_{11} = 1 + \dfrac{i}{K}$, $\theta = \arctan\dfrac{1}{K} = \arctan\dfrac{m\alpha}{\hbar^2 k}$ and the equation for resonances ($T = 1$) is

$$\tan kL = -\frac{\hbar^2 k}{m\alpha}. \tag{1.52}$$

Close to the resonance, around one of the resonance energies E_n, the transmission coefficient has a *Lorentzian* form

$$T(E) \approx \frac{\Gamma_n^2}{(E - E_n)^2 + \Gamma_n^2}, \tag{1.53}$$

where the width Γ_n is given for two δ-barriers as

$$\Gamma_n = \left(\frac{2\hbar^2 E_n T_1^2}{mL^2 R_1}\right)^{1/2}. \tag{1.54}$$

1.2 Landauer formula

1.2.1 Single-channel formulas

The main idea of the scattering approach to the conductance was first formulated by Rolf Landauer [1, 2]. He proposed, that the conductance of some segment of a 1D channel with elastic scatterers is determined by the quantum mechanical probabilities of transmission (T) and reflection $(R = 1 - T)$ through this segment. It should be noted, that Landauer considered the local resistance of a system (the zero-temperature residual resistance), but not the resistance of a quantum system between two equilibrium electrodes. As a result, he got for the zero temperature one-channel (effectively one-dimensional) conductance the so-called "first Landauer formula"

$$G' = \frac{e^2}{h} \frac{T}{1-T} = \frac{e^2}{h} \frac{T}{R}. \qquad (1.55)$$

The result, which seems to be reasonable at least in two limiting cases. At small transmission $T \to 0$, the conductance is also small and proportional to T, the result, which is well known from the perturbation theory. In the opposite case, when $T \to 1$, $R \to 0$, there is no scattering at all, so that the conductance should go to infinity, in agreement with (1.55). To take into account the spin degeneracy in this formula, one has to multiply the conductance (1.55) by 2.

However, the further investigations [3, 4] show that the conductance of a 1D system, calculated by the exact linear response method, can have also quite different form (depending on the boundary conditions)

$$G = \frac{e^2}{h} T. \qquad (1.56)$$

This conductance is finite even in the case of the perfectly transmitted junction $(T = 1)$. Actually, there is no contradiction between these two formulas. It was shown that both are reasonable and give the same current, but correspond to the voltages, defined between different points. As we shall see below, the key difference between the formulas (1.55) and (1.56) is that the first one is for the conductance *inside* the junction (between points A and B, see Fig. 1.9 below), while the second gives the conductane related to the equilibrium electrodes (between points L and R in the Fig. 1.9). In the section 1.2.4 we obtain both formulas and discuss the relation between them. The puzzle with finite resistance at $T \to 1$ is also understood, it is clear now that the current through a junction is always accompanied by the voltage drop at the boundaries between electrodes and leads. The physical reason is that the number of open electron transport channels is limited, while many other electrons reflect from the junction and create some charge distribution. Not so obvious is, however, that this contact resistance has the universal value $R_c = h/e$ for one spinless channel.

For the transport problems, considered in this book, the second type of the Landauer formula is more important usually. Besides, the first type formulas are not exact for finite-size nanostructures, because they are dependent on the particular electrical potential distribution inside the junction.

The important question, discussed in connection with the Landauer resistance, is the origin of dissipation in this approach. Indeed, finite dc current at finite dc voltage means that the energy is permanently dissipated. On the other hand, we consider only elastic scattering, so that the energy can not be dissipated in the scattering process. This problem is closely related to the phenomena of the residual resistance at low temperature, caused by impurities. In both cases we should introduce some thermalisation. In the case of transport between the *equilibrium* electrodes, this problem is resolved quite easy, the energy is dissipated in the electrodes, the details of the dissipation are not relevant. More precisely, the *incoming* from the electrodes particles are equilibrium distributed, while *outgoing* particles propagate into the electrodes and are thermalised here.

At finite temperature and finite voltage the Landauer formula (1.56) is transformed into the more general formula for the current:

$$I(V) = \frac{e}{h} \int_{-\infty}^{\infty} T(E,V) \left[f_0(E + eV) - f_0(E) \right] dE, \tag{1.57}$$

where $f^0(E)$ is the Fermi-Dirac distribution function with the Fermi energy ε_F:

$$f_0(E) = \frac{1}{\exp\left(\frac{E - \varepsilon_F}{T} \right) + 1}. \tag{1.58}$$

1.2.2 Heuristic derivation

Now we are ready to see in detail, how the transmission coefficient can be used to calculate the current through a quantum junction. We start from the mode-conserving scattering and use here the heuristic arguments. More rigorous methods are summarized in section 1.3.

From the scattering picture it follows that all particles, coming from the left electrode, are transmitted through the junction with the probability $T(n, k_z)$ and, after that, their excess energy, phase coherence, and the memory of their previous state are lost in the right electrode. We assume in all cases, that an electron can go without scattering from the lead into the electrode, thus for incoming from the left electrons there are only two possibilities: to go into right electrode with the probability T or to return back to the left electrode with the probability R. The same property takes place for all particles coming from the right and transmitted to the left. Transport through the junction is coherent in this model, energy E and transverse quantum number n are conserved (the case of the multi-channel scattering, when n is not conserved, will be considered later). Irreversibility is introduced through the relaxation in the electrodes. The main assumption is that *the right-moving particles in the left lead are populated with the equilibrium distribution function of the left electrode* $f_L^{eq}(E)$ and *the left-moving particles in the right lead are populated with the equilibrium distribution function of the right electrode* $f_R^{eq}(E)$ (see Fig. 1.7).

According to this model, the current of electrons, which enter from the left electrode is determined by the following exspression

$$J_{L \to R} = e \sum_n \int_0^\infty T_{L \to R}(n, k_z) v_L(n, k_z) f_L(n, k_z) \frac{dk_z}{2\pi}, \qquad (1.59)$$

where $v_L(n, k_z)$ is the group velocity of the particle with momentum k_z, $f_L(n, k_z)$ is the distribution function, the form of this function is considered below. The integration is only for right-moving particles with $k_z > 0$. Note, that it is not necessary to multiply this expression additionally by the factor like $(1 - f_R((n, k_z))$ as in the tunneling "golden rule" theory, because this factor describes the number of empty states in the right equilibrium electrode and should be included when the transition between left and right states is considered. Instead, in our approach we consider *scattering states in the leads*, which formally can be extended in the electrodes. The transmission coefficient from the left to the right is simply the probability to find a particle in the right part of this state.

Taking into account that

$$v(k_z) = \frac{\partial E_z(k_z)}{\hbar \partial k_z} = \frac{\partial E(k_z)}{\hbar \partial k_z}, \qquad (1.60)$$

where $E(k_z) = E_n + E_z(k_z)$ is the full energy, we obtain

$$I_{L \to R} = \frac{e}{h} \sum_n \int_{E_{nL}}^\infty T_{L \to R}(n, E) f_L(E) dE, \qquad (1.61)$$

and similar expression for the current of right-incoming electrons

$$I_{R \to L} = \frac{e}{h} \sum_n \int_{E_{nR}}^\infty T_{R \to L}(n, E) f_R(E) dE. \qquad (1.62)$$

Note that the integration in this expressions is done from the bottom of conduction band $E_{nL(R)}$. Taking into account the symmetry of transmission coefficients (1.22) we get the expression for the current

$$I = \frac{e}{h} \sum_n \int_{-\infty}^\infty T_n(E) \left[f_L^{eq}(E) - f_R^{eq}(E) \right] dE. \qquad (1.63)$$
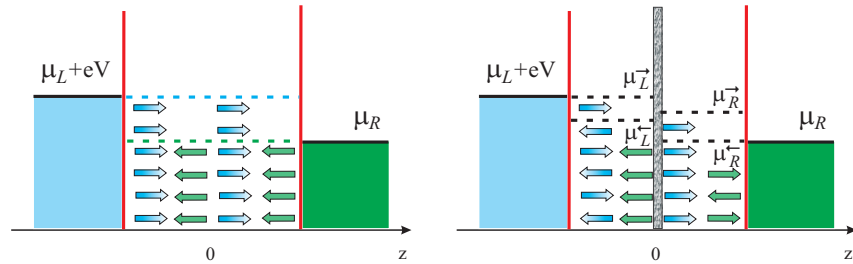

Fig. 1.7. Left-moving and right-moving particles in a perfect wire (left) and in a wire with scatterer (energy diagram).

The limits of integration over E can be taken infinite, because the closed channels have $T_n(E) = 0$ and do not contribute to the current.

Finally, the distribution functions in this expression should be discussed. There are different possibilities to create a nonequilibrium state of the junction. In equilibrium the *electro-chemical potential* $\tilde{\mu} = \mu + e\varphi$ should be the same in both electrodes. Here μ is the *(internal) chemical potential*, which determines the filling of electron bands in the electrodes, and φ is the electrostatic potential. One can create a difference of only (internal) chemical potentials (Fig. 1.8, left) if populates one of the electrodes with extra particles. This case, however, is quite difficult to realize in nanostructures, because any change of the particle density causes the change in the electric field. Moreover, typically the external voltage is applied to the electrodes, while the (internal) chemical potentials of the electrodes far from the junction are not changed, $\mu_L = \mu_R = \mu$ (Fig. 1.8, right). More generally, one can say that the difference in the electro-chemical potentials between two points taken inside the equilibrium electrodes, is always produced by the external voltage ($\tilde{\mu}_L - \tilde{\mu}_R = eV$). To determine the exact distribution of the charge density and electrostatic potential near and inside the junction, the self-consistent solution of the coupled Schrödinger and Poisson equations is necessary. In this case the expression (1.63) should be used with care when the voltage is not small. Indeed, the potential $U(z)$ is now a function of the applied voltage, and consequently the transmission coefficient is a function of the voltage too.

The distribution functions in the general case are

$$f_L^0(E) = \frac{1}{\exp\left(\frac{E - \mu_L - e\varphi_L}{T}\right) + 1}, \quad f_R^0(E) = \frac{1}{\exp\left(\frac{E - \mu_R - e\varphi_R}{T}\right) + 1}. \qquad (1.64)$$

But usually the simplified form can be used, with explicitly written external voltage

$$I(V) = \frac{e}{h} \sum_n \int_{-\infty}^{\infty} T_n(E, V) \left[f_0(E + eV) - f_0(E)\right] dE. \qquad (1.65)$$

Where $f^0(E)$ is the Fermi-Dirac distribution function with the equilibrium chemical potentials $\mu_L = \mu_R = \varepsilon_F$:
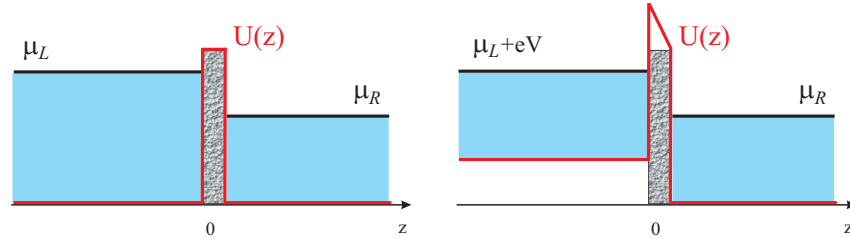

Fig. 1.8. Energy diagrams for chemical potential difference (left picture, the number of electrons in the band is changed, but not the potential) and voltage difference (right picture, the electron band is shifted up, the potential is modified).

$$f_0(E) = \frac{1}{\exp\left(\frac{E-\varepsilon_F}{T}\right)+1}. \tag{1.66}$$

The distribution functions in the electrodes are the functions of energy E only, thus one can introduce *the transmission function*

$$\bar{T}(E) = \sum_n T_n(E). \tag{1.67}$$

and obtain finally

$$I(V) = \frac{e}{h} \int_{-\infty}^{\infty} \bar{T}(E,V)\left[f_0(E+eV) - f_0(E)\right] dE. \tag{1.68}$$

This formula can be wrong, however, if the external magnetic field is applied, because the magnetic field violates the time-reversal symmetry and the relation (1.22) may be violated too.

The conductance at zero temperature is

$$G = \frac{e^2}{h} \sum_n T_n(\varepsilon_F). \tag{1.69}$$

1.2.3 Conductance quantization

Perfect wire

Consider now the conductance of a perfect wire adiabatically coupled to two electrodes. "Perfect wire" means that there are several open reflectionless channels with transmission coefficient $T_n(E) = 1$. Thus all right going electrons inside the junction are populated only by the left electrode and left-going electrons are populated only by the right elecrode (Fig. 1.7, left). We can say that right moving electrons have the (pseudo-) electro-chemical potential of the left elecrode $\tilde{\mu}_L$, while left moving electrons of the right electrode $\tilde{\mu}_R$. Of course, the state of electrons inside the wire is not equilibrium, and these "left" and "right" chemical potentials give the number and energy of corresponding particles in the channel, but they are not usual thermodynamic potentials.

Now we simply use the expression for the current (1.68). The distribution functions in the electrodes at zero-temperature are the step-functions

$$f_L(E,V) = \theta(\mu + eV - E), \tag{1.70}$$
$$f_R(E) = \theta(\mu - E), \tag{1.71}$$

and for the current we obtain

$$I(V) = \frac{e}{h} \sum_n \int_{-\infty}^{\infty} T_n(E,V)\left[\theta(\mu + eV - E) - \theta(\mu - E)\right] dE =$$
$$= \frac{e}{h} \sum_n \int_{\mu - E_n}^{\mu - E_n + eV} T_n(E,V) dE = \frac{e^2}{h} NV, \tag{1.72}$$

where we used $T_n(E,V) = 1$, and N is the number of open channels between $\tilde{\mu}_L = \mu + eV$ and $\tilde{\mu}_R = \mu$. For the conductance one has

$$G = \frac{e^2}{h}N. \tag{1.73}$$

It is accepted to call the conductance of a single-channel perfect wire with spin as *the conductance quantum*

$$G_0 = \frac{2e^2}{h} \approx 77.48\ \mu S = 7.748 \cdot 10^{-5}\ \Omega^{-1} \approx \frac{1}{12900}\ \Omega^{-1}. \tag{1.74}$$

The corresponding resistance is

$$R_0 = \frac{h}{2e^2} = 12.9\ k\Omega. \tag{1.75}$$

Where does the resistance of a *perfect* wire come from? The origin of this resistance is in the mismatch between the large number of modes in the electrodes and a few channels in the wire. So this is not the resistance of a perfect wire, but rather the contact resistance of the interface between electrodes and wire.

Quantum point contact

In quantum point contacts (QPC), which have usually the adiabatic form, the conductance at low temperatures is quantized in accordance with (1.73). In the spin-degenerate case it can be written as,

$$G = \frac{2e^2}{h}\sum_n \theta(E_F - E_n), \tag{1.76}$$

where E_F is the Fermi energy, and E_n is the maximum of the transverse energy $E_n(z)$. The Fermi energy in 2D electron gas can be changed by the gate voltage V_g, in this way the conductance quantization was observed experimentally in the form of steps at the function $G(V_g)$.

At finite temperature the conductance steps are smeared. Besides, the steps are not perfect, if the junction is not adiabatic. This can be seen from the exactly solvable model with the potential

$$V(x,z) = \frac{1}{2}m\omega_x^2 x^2 + V_0 - \frac{1}{2}m\omega_z^2 z^2. \tag{1.77}$$

The transmission coefficients have a simple form [5]:

$$T_n(E) = \frac{1}{\exp\left[-2\pi\left(E - V_0 - (n+1/2)\hbar\omega_x\right)/(\hbar\omega_z)\right] + 1}. \tag{1.78}$$

At $\omega_z \ll \omega_x$ we return to the adiabatic approximation and well defined steps.

Classical point contact

It is interesting to compare the quantum conductance (1.73) with the conductance of a *classical* point contact with large width $d_0 \gg \lambda_F$, known as Sharvin conductance [6]. Following [7], this conductance for 2D ballistic channel with the width d_0 between two Fermi gases can be written as

$$I = \frac{e\upsilon_F}{\pi} d_0 \frac{\partial n}{\partial \mu} eV, \tag{1.79}$$

In 2D electron gas $\partial n/\partial \mu = m/\pi\hbar^2$, and we obtain (with spin degeneracy)

$$G_S = \frac{2e^2}{h} \frac{k_F d_0}{\pi}. \tag{1.80}$$

From quantum mechanical point of view $k_F d_0/\pi$ is the number of transverse channels N.

1.2.4 Contact resistance

Consider now the single-channel case with the imperfect transmission $T \neq 1$, repeating the same calculation as in (1.72) we obtain

$$I = \frac{e}{h} T \left(\tilde{\mu}_L - \tilde{\mu}_R \right) = \frac{e^2}{h} TV, \tag{1.81}$$

$$G = \frac{e^2}{h} T. \tag{1.82}$$

This is the conductance between the reservoirs, e.g. between some two points "L" and "R" inside the electrodes (see Fig. 1.9). Now consider two other points "A" and "B" *inside the leads*. The distribution functions and corresponding "electro-chemical potentials" (these potentials are not true potentials, but give the correct number and energy of electrons, as we discussed before) are different for left and right moving
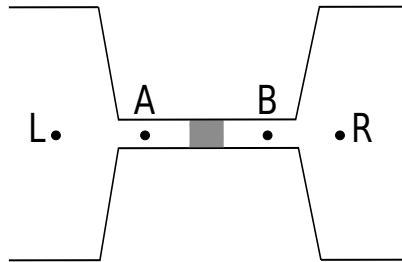

Fig. 1.9. The points of voltage measurement: L,R in the equilibrium electrodes; A,B inside the leads.

electrons. Now, however, these potentials are different also at different sides of the scatterer (Fig. 1.7, right). The potential $\tilde{\mu}_L^{\rightarrow}$ of the right moving electrons is equal to $\tilde{\mu}_L$ only in the left part of the wire, as well as $\tilde{\mu}_R^{\leftarrow} = \tilde{\mu}_R$ in the right part. All other electro-chemical potentials are modified by the reflection from the barrier. Assume, that one can approximate the charge redistribution in the leads due to scattering by some quasiequilibrium distributions with corrsponding pseudo-potentials $\tilde{\mu}$. For example, only the part of right moving electrons is transmitted through the barrier and corresponding potential should be $T\tilde{\mu}_L$, but additionally $(1-T)\tilde{\mu}_R$ are reflected and move back. Finally, we obtain

$$\tilde{\mu}_L^{\rightarrow} = \tilde{\mu}_L, \quad \tilde{\mu}_R^{\rightarrow} = T\tilde{\mu}_L + (1-T)\tilde{\mu}_R, \tag{1.83}$$
$$\tilde{\mu}_R^{\leftarrow} = \tilde{\mu}_R, \quad \tilde{\mu}_L^{\leftarrow} = T\tilde{\mu}_R + (1-T)\tilde{\mu}_L. \tag{1.84}$$

The *difference* of both "left moving" and "right moving" chemical potentials across the barrier is the same

$$\tilde{\mu}_L^{\rightarrow} - \tilde{\mu}_R^{\rightarrow} = \tilde{\mu}_L^{\leftarrow} - \tilde{\mu}_R^{\leftarrow} = (1-T)(\tilde{\mu}_L - \tilde{\mu}_R). \tag{1.85}$$

We can identify this potential difference with the potential drop between points A and B

$$eV_{AB} = (1-T)(\tilde{\mu}_L - \tilde{\mu}_R). \tag{1.86}$$

Thus we can define the conductance (with the current (1.81))

$$G' = \frac{I}{V_{AB}} = \frac{e^2}{h}\frac{T}{1-T} = \frac{e^2}{h}\frac{T}{R}, \tag{1.87}$$

which is exactly "the first Landauer formula" (1.55). The voltage V_{AB} appears as a result of charge redistribution around the scatterer. Not surprising that for perfect wire with $T = 1$ and $R = 0$ this conductance is infinite.

The conductances (1.82) and (1.87) obey the following relation:

$$\frac{1}{G} = \frac{h}{e^2} + \frac{1}{G'}. \tag{1.88}$$

This result can be understood in the following way. G^{-1} can be considered as the full resistance of the junction, consisted from two sequential resistances of the scatterer (G'^{-1}) and of the contact resistance of the perfect wire (h/e^2).

Consider additionally the conductance of the *incoherent* series of N scatterers, each having the transmission coefficient T_1. If the phase coherence is broken, one should summarize the probabilities of transmission instead of the quantum amplitudes. Thus, the transfer matrix method does not work i this case. Instead we use the probability theory. Let us consider first only two scatterers with the transmission coefficients T_1 and T_2. The probability of transmission trough both scatterers T is calculated as the sum of all possible (re)scattering processes

$$T = T_1T_2 + T_1R_2R_1T_2 + T_1R_2R_1R_2R_1T_2 + ...$$
$$= T_1(1 + R_1R_2 + (R_1R_2)^2 + ...)T_2 = \frac{T_1T_2}{1 - R_1R_2}, \tag{1.89}$$

or

$$\frac{1-T}{T} = \frac{1-T_1}{T_1} + \frac{1-T_2}{T_2}, \tag{1.90}$$

which demonstrates the additivity of $(1-T)/T$. Thus, for N scatterers we obtain

$$\frac{1-T}{T} = N\frac{1-T_1}{T_1}. \tag{1.91}$$

The resistance of the system is

$$R = \frac{h}{e^2}\frac{1}{T} = \frac{h}{e^2} + N\frac{h}{e^2}\frac{R_1}{T_1}. \tag{1.92}$$

We again obtain the series resistance of N Landauer scatterers and contact resistance.

1.3 Multi-channel scattering and transport

1.3.1 $\hat{S}$-matrix and scattering states

Consider now the general multi-channel case, when the scattering is possible between different modes. It is convenient to define separately left (L) and right (R), incoming (+) and outgoing (-) modes (Fig. 1.10). We assume that at $z < z_L$ and $z > z_R$ the leads have a constant cross-sections. To make the $\hat{S}$-matrix unitary, we introduce the normalization of incoming and outgoing modes, as was discussed in sec. 1.1.4. Thus, outside the scattering region we define

$$\psi_{LnE}^+(\mathbf{r}) = \frac{1}{\sqrt{2\pi\hbar v_{Ln}}}\phi_{Ln}(x,y)A_{n+}e^{ik_n z}, \quad z < z_L \tag{1.93}$$

$$\psi_{LnE}^-(\mathbf{r}) = \frac{1}{\sqrt{2\pi\hbar v_{Ln}}}\phi_{Ln}(x,y)A_{n-}e^{-k_n z}, \quad z < z_L \tag{1.94}$$

$$\psi_{RmE}^+(\mathbf{r}) = \frac{1}{\sqrt{2\pi\hbar v_{Rm}}}\phi_{Rm}(x,y)B_{m+}e^{-ik_m' z}, \quad z > z_R \tag{1.95}$$

$$\psi_{RmE}^-(\mathbf{r}) = \frac{1}{\sqrt{2\pi\hbar v_{Rm}}}\phi_{Rm}(x,y)B_{m-}e^{ik_m' z}, \quad z > z_R. \tag{1.96}$$
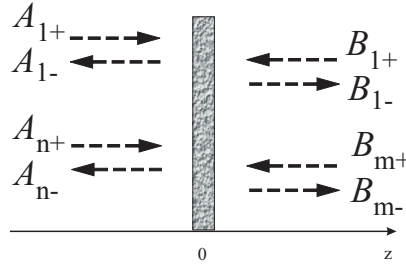
Fig. 1.10. Multi-channel scattering.

Here n and m label the left and right transport channels respectively, $\phi_{Ln}(x,y)$ and $\phi_{Rm}(x,y)$ are the left and right transverse eigenfunctions, $\upsilon_{Ln} = \hbar k_n/m_L$ and $\upsilon_{Rm} = \hbar k'_m/m_R$ are the velocities, $\hbar k_n = \sqrt{2m_L(E - E_n)}$, $\hbar k'_m = \sqrt{2m_R(E - E_m)}$, E_n, E_m being transverse eigenenergies. As in the single-channel case, we mark the left wave amplitudes with $A_\pm$ and right with $B_\pm$.

The initial incoming states become now

$$\psi^{in}_{L(R)nE}(\mathbf{r}) = \frac{1}{\sqrt{2\pi\hbar\upsilon_{L(R)n}}}\phi_{L(R)n}(x,y)e^{+(-)ik_n z}. \tag{1.97}$$

It is important to remember, that we change the normalization, but we must keep the density of states. Indeed, the matrix element $\langle \psi^{in}_{nE}|\psi^{in}_{nE}\rangle$ acquires the additional multiplier $1/(h\upsilon)$. Thus, we should change

$$\int \frac{dk}{2\pi} = \int \frac{dE}{h\upsilon} \quad \Rightarrow \int \frac{dk}{2\pi}h\upsilon = \int dE. \tag{1.98}$$

This integration rule follows also from the normalization condition

$$\langle \psi^{in}_{L(R)nE}|\psi^{in}_{L(R)n'E'}\rangle = \int \left(\psi^{in}_{L(R)nE}(\mathbf{r})\right)^* \psi^{in}_{L(R)n'E'}(\mathbf{r})dxdydz = \delta_{nn'}\delta(E - E'). \tag{1.99}$$

Scattering matrix relates *all incoming* with *all outgoing* modes. In the single-channel case, considered previously, $\hat{S}$ is 2×2 matrix (1.31). In the general multi-channel case the $\hat{S}$-matrix is defined as $N \times N$ matrix

$$\begin{pmatrix} A_{1-} \\ \dots \\ A_{N_L-} \\ B_{1-} \\ \dots \\ B_{N_R-} \end{pmatrix} = \hat{S}\begin{pmatrix} A_{1+} \\ \dots \\ A_{N_L+} \\ B_{1+} \\ \dots \\ B_{N_R+} \end{pmatrix} = \begin{pmatrix} S_{11} & S_{12} & \dots & S_{1N} \\ S_{21} & S_{22} & \dots & S_{2N} \\ \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots \\ S_{N1} & S_{N2} & \dots & S_{NN} \end{pmatrix}\begin{pmatrix} A_{1+} \\ \dots \\ A_{N_L+} \\ B_{1+} \\ \dots \\ B_{N_R+} \end{pmatrix}, \tag{1.100}$$

where N_L and N_R are the numbers of left and right channels, $N = N_L + N_R$.

We represent it in the block form, analogous to (1.31):

$$\hat{S} = \begin{pmatrix} \hat{r} & \hat{t}' \\ \hat{t} & \hat{r}' \end{pmatrix} \tag{1.101}$$

where the matrices $\hat{r}$ ($N_L \times N_L$) and $\hat{t}$ ($N_L \times N_R$) describe transmission and reflection of the states incoming from the left, the matrices $\hat{r}'$ ($N_R \times N_R$) and $\hat{t}'$ ($N_R \times N_L$) describe transmission and reflection of the states incoming from the right, N_L (N_R) is the number of the left (right) channels.

The matrix $\hat{t}$ is called *transmission matrix*, $T_{mn} = |t_{mn}|^2$ are the probabilities of transmission from the left mode n into the right mode m, $R_{n'n} = |r_{n'n}|^2$ are the probabilities of reflection from the left mode n into the left mode n', etc.

The scattering marix is unitary

$$\hat{S}^\dagger\hat{S} = \hat{S}\hat{S}^\dagger = \hat{I}, \tag{1.102}$$

from which the conservation of total probability is clear

$$\left(\hat{S}^{\dagger}\hat{S}\right)_{nn} = \sum_{n'}|r_{nn'}|^2 + \sum_{m}|t_{nm}|^2 = 1. \tag{1.103}$$

The other useful relations are

$$\hat{r}^{\dagger}\hat{r} + \hat{t}^{\dagger}\hat{t} = \hat{r}'^{\dagger}\hat{r}' + \hat{t}'^{\dagger}\hat{t}' = \hat{I}, \tag{1.104}$$

$$\hat{r}\hat{r}^{\dagger} + \hat{t}'\hat{t}'^{\dagger} = \hat{r}'\hat{r}'^{\dagger} + \hat{t}\hat{t}^{\dagger} = \hat{I}, \tag{1.105}$$

$$\hat{r}^{\dagger}\hat{t}' + \hat{t}^{\dagger}\hat{r}' = \hat{t}'^{\dagger}\hat{r} + \hat{r}'^{\dagger}\hat{t} = 0, \tag{1.106}$$

$$\hat{r}\hat{t}^{\dagger} + \hat{t}'\hat{r}'^{\dagger} = \hat{t}\hat{r}^{\dagger} + \hat{r}'\hat{t}'^{\dagger} = 0. \tag{1.107}$$

From which follows

$$\mathrm{Tr}\left(\hat{t}^{\dagger}\hat{t}\right) = \mathrm{Tr}\left(\hat{t}\hat{t}^{\dagger}\right) = \mathrm{Tr}\left(\hat{t}'^{\dagger}\hat{t}'\right) = \mathrm{Tr}\left(\hat{t}'\hat{t}'^{\dagger}\right), \tag{1.108}$$

$$\mathrm{Tr}\left(\hat{r}^{\dagger}\hat{r}\right) = \mathrm{Tr}\left(\hat{r}\hat{r}^{\dagger}\right) = \mathrm{Tr}\left(\hat{r}'^{\dagger}\hat{r}'\right) = \mathrm{Tr}\left(\hat{r}'\hat{r}'^{\dagger}\right). \tag{1.109}$$

In the time-reversal case the $\hat{S}$-matrix is symmetric

$$\hat{S} = \hat{S}^{T}, \tag{1.110}$$

thus the reflection matrix is also symmetric $r_{nn'} = r_{n'n}$, and $\hat{t}' = \hat{t}^{T}$.

In the external magnetic field more general conditions take place:

$$r_{nn'}(B) = r_{n'n}(-B), \tag{1.111}$$

$$t_{nm}(B) = t'_{mn}(-B). \tag{1.112}$$

The simplest way to proceed is to use the so-called scattering states. Using incoming and outgoing modes in the right and left leads (1.93)-(1.96), we can define the scattering states as

$$\Psi_{LnE}(\mathbf{r}) = \begin{cases} \dfrac{1}{\sqrt{2\pi\hbar v_{Ln}}}\phi_{Ln}(x,y)e^{ik_n z} + \sum_{n'}\dfrac{r_{n'n}}{\sqrt{2\pi\hbar v_{Ln'}}}\phi_{Ln'}(x,y)e^{-ik_n z},\ z < z_L, \\[3mm] \sum_{m}\dfrac{t_{mn}}{\sqrt{2\pi\hbar v_{Rm}}}\phi_{Rm}(x,y)e^{ik'_m z},\ z > z_R. \end{cases}$$

$$\tag{1.113}$$

The physical sense of this state is quite transparent. It describes a particle moving from the left and splitting into reflected and transmitted parts. We established that it is important for Landauer transport, that only these states are populated from the left reservoir, so that one can accept the distribution of "left" scattering states to be equilibrium with the left electro-chemical potential. The "right" states, populated by the right reservoir, are defined as

$$\Psi_{RmE}(\mathbf{r}) = \begin{cases} \dfrac{1}{\sqrt{2\pi\hbar v_{Rm}}}\phi_{Rm}(x,y)e^{-ik'_m z} + \sum_{m'}\dfrac{r'_{m'm}}{\sqrt{2\pi\hbar v_{Rm'}}}\phi_{Rm'}(x,y)e^{ik'_m z},\ z > z_R, \\[3mm] \sum_{n}\dfrac{t'_{nm}}{\sqrt{2\pi\hbar v_{Ln}}}\phi_{Ln}(x,y)e^{-ik_n z},\ z < z_L. \end{cases}$$

$$\tag{1.114}$$

Now, using the left and right states(1.93)-(1.96) or the scattering states (1.113), (1.114), it is straightforward to obtain the Landauer formula.

1.3.2 Multi-channel Landauer formula

Below in the section 1.3 we consider only time-reversal case, so that

$$R_{n'n} = |r_{n'n}|^2 = |r_{nn'}|^2 = R_{nn'},\qquad(1.115)$$

$$T_{mn} = |t_{mn}|^2 = |t'_{nm}|^2 = T'_{nm}.\qquad(1.116)$$

Zero temperature conductance

The heuristic calculation of the conductance is straightforward. The current from the left mode $\psi_{Ln}^+(\mathbf{r})$ into the right mode $\psi_{Rm}^-(\mathbf{r})$ is determined by the transmission probability T_{mn}. The inverse current from $\psi_{Ln}^-(\mathbf{r})$ into $\psi_{Rm}^+(\mathbf{r})$ is determined by $T'_{nm} = T_{mn}$. Assuming that all left states $\psi_{Ln}^+(\mathbf{r})$ are populated with the electrochemical potential of the left electrode, and right states $\psi_{Rm}^-(\mathbf{r})$ are populated with the electrochemical potential of the right electrode, we obtain the current of incoming left n and right m electrons as

$$I_{mn} = \frac{e}{h} T_{mn} \left(\tilde{\mu}_L - \tilde{\mu}_R \right),\qquad(1.117)$$

summing contributions from all incoming left modes and all incoming right modes we obtain the full current

$$I = \frac{e}{h} \sum_{n=1}^{N_L} \sum_{m=1}^{N_R} T_{mn} \left(\tilde{\mu}_L - \tilde{\mu}_R \right).\qquad(1.118)$$

After the obvious mathematical transformation

$$\sum_{n=1}^{N_L} \sum_{m=1}^{N_R} T_{mn} = \sum_{n=1}^{N_L} \sum_{m=1}^{N_R} |t_{mn}|^2 = \sum_{n=1}^{N_L} \sum_{m=1}^{N_R} t_{mn} t_{mn}^* = \sum_{n=1}^{N_L} \sum_{m=1}^{N_R} \left(\hat{t}^\dagger \right)_{nm} t_{mn}$$

$$= \sum_{n=1}^{N_L} \left(\hat{t}^\dagger \hat{t} \right)_{nn} = \mathrm{Tr}\left(\hat{t}^\dagger \hat{t} \right),\qquad(1.119)$$

we obtain the Landauer multichannel current and conductance

$$I = \frac{e}{h} \mathrm{Tr}\left(\hat{t}^\dagger \hat{t} \right) \left(\tilde{\mu}_L - \tilde{\mu}_R \right) = \frac{e^2}{h} \mathrm{Tr}\left(\hat{t}^\dagger \hat{t} \right) V,\qquad(1.120)$$

$$G = \frac{e^2}{h} \mathrm{Tr}\left(\hat{t}^\dagger \hat{t} \right).\qquad(1.121)$$

General expression

If we repeat the above summation procedure at finite temperature and voltage, we obtain a generalized form of the equation (1.63)

$$I(V) = \frac{e}{h} \sum_{nm} \int_{-\infty}^{\infty} T_{nm}(E,V) \left[f_L(E) - f_R(E) \right] dE.\qquad(1.122)$$

It is instructive, however, to consider an approach utilizing the scattering states. Let us calculate the current carrying by one scattering state $\Psi_{LnE}(\mathbf{r})$ (1.113). Direct application of the current density expression

$$\mathbf{j} = \frac{ie\hbar}{2m}\left[\psi(\mathbf{r})\nabla\psi^*(\mathbf{r}) - \psi^*(\mathbf{r})\nabla\psi(\mathbf{r})\right] \tag{1.123}$$

gives the following answer for the z-component of the current density:

$$j_{LnE}^z = \frac{ie\hbar}{2m}\sum_{mm'}\frac{t_{mn}t_{m'n}^*}{2\pi\hbar\sqrt{v_{Rm}v_{Rm'}}}\phi_{Rm}(x,y)\phi_{Rm'}^*(x,y)(-ik_{m'}' - ik_m')e^{ik_m'z - ik_{m'}'z} \tag{1.124}$$

And integrating over (x,y) and using the orthogonality property

$$\int\int\phi_{Rm}(x,y)\phi_{Rm'}(x,y)dxdy = \delta_{mm'}, \tag{1.125}$$

we get

$$I_{LnE} = e\sum_m |t_{mn}|^2 = \frac{e}{h}\left(\hat{t}^\dagger\hat{t}\right)_{nn}. \tag{1.126}$$

We can summarize over transport channels, and obtain the following general two-terminal Landauer formula for the current

$$I(V) = \frac{e}{h}\int_{-\infty}^{\infty}\overline{T}(E,V)\left[f_0(E + eV) - f_0(E)\right]dE, \tag{1.127}$$

with

$$\overline{T}(E,V) = \sum_n\left(\hat{t}^\dagger\hat{t}\right)_{nn} = \mathrm{Tr}\left(\hat{t}^\dagger\hat{t}\right) = \sum_{nm}T_{mn}. \tag{1.128}$$

$\overline{T}(E,V)$ is the effective *transmission function* for the particles with the energy E. The most important advantage of this formula is, that the transmission function can be calculated from the quantum scattering theory. Thus, the kinetic problem is reduced to the pure quantum mechanical problem of a single particle in a static potential. The formula (1.127) is the most general *two-terminal* formula. All other Landauer formulas can be obtained in the limiting cases from (1.127). For the finite-temperature conductance we have

$$G = \frac{e^2}{h}\int_{-\infty}^{\infty}\overline{T}(E)\left(-\frac{\partial f_0}{\partial E}\right)dE. \tag{1.129}$$

At zero temperature $(-\partial f_0/\partial E) = \delta(E - E_F)$, thus

$$G = \frac{e^2}{h}\overline{T}(E_F). \tag{1.130}$$

In agreement with the previous results.

Transmission probabilities and transmission eigenvalues

The physical sense of the transmission function (1.128) can be interpreted in two different ways.

First, $T_n = \left(\hat{t}^\dagger \hat{t}\right)_{nn}$ is the transmission probability for the incoming state in the n-th channel.

On the other hand, the $N \times N$ matrix $\hat{t}^\dagger \hat{t}$ can be diagonalized. One can consider the eigenvalues $\mathscr{T}_n$ as the transmission coefficients in the basis of independent transport channels.

The conductance has the same form in both cases because of the invariance of the trace

$$G = \frac{e^2}{h} \sum_n T_n = \frac{e^2}{h} \sum_n \mathscr{T}_n. \qquad (1.131)$$

1.3.3 Derivation from the linear response theory

In the previous sections we obtained the Landauer formula, valid at finite voltage, using some additional arguments about the populations of the states inside the junction. Here we restrict ourselves by the linear response approach, which is valid only in the limit of small voltage, but is exact.

We start from the Kubo formula for conductance (we follow Bruus and Flensberg [8]):

$$G = \lim_{\omega \to 0} \frac{\hbar}{\omega} \mathrm{Re} \int_0^\infty dt\, e^{i(\omega + i\eta)t} \left\langle \left[\hat{I}(t), \hat{I}(0)\right]_- \right\rangle_{eq}, \qquad (1.132)$$

where $[...]_-$ is the commutator, the matrix elements of the current operator $\hat{I}$ in the Hilbert space of single particle eigenfunctions $\Psi_\lambda(\mathbf{r})$ are

$$I_{\lambda\lambda'}(z) = \frac{ie\hbar}{2m} \int dx dy \left(\Psi_\lambda \frac{\partial \Psi_{\lambda'}^*}{\partial z} - \Psi_{\lambda'}^* \frac{\partial \Psi_\lambda}{\partial z} \right), \qquad (1.133)$$

which should be independent of z in the stationary case because of current conservation, and can be evaluated at any cross-section.

To proceed, we use the current operators in the second quantization representation:

$$\hat{I} = \sum_{\lambda\lambda'} I_{\lambda\lambda'} c_\lambda^\dagger c_{\lambda'}, \qquad (1.134)$$

and choose the scattering states (1.113), (1.114) as eigenfunctions Ψ_λ with λ being equivalent to the set s, n, E, where $s = L, R$ is the lead index, n is the number of channel in the lead s, and E is the energy. Straightforward calculation of the statistical average in equilibrium, using $\left\langle c_\lambda^\dagger c_{\lambda'} \right\rangle_{eq} = f_0(E_\lambda)\delta_{\lambda\lambda'}$ and $I_{\lambda\lambda'} = I_{\lambda'\lambda}^*$, gives

$$\left\langle \left[\hat{I}(t), \hat{I}(0)\right]_- \right\rangle_{eq} = \sum_{\lambda\lambda'\mu\mu'} I_{\mu\mu'} I_{\lambda\lambda'} e^{i(E_\lambda - E_{\lambda'})} \left\langle \left[c_\lambda^\dagger c_{\lambda'}, c_\mu^\dagger c_{\mu'}\right]_- \right\rangle_{eq}$$

$$= \sum_{\lambda\lambda'} |I_{\lambda\lambda'}|^2 e^{i(E_\lambda - E_{\lambda'})} \left[f_0(E_\lambda) - f_0(E_{\lambda'}) \right]. \qquad (1.135)$$

Inserting this into (1.132) and integrating, we get

$$G = \lim_{\omega \to 0} \frac{\hbar}{\omega} \operatorname{Im} \sum_{\lambda \lambda'} \frac{|I_{\lambda \lambda'}|^2}{\omega + i\eta + E_\lambda - E_{\lambda'}} \left[f_0(E_\lambda) - f_0(E_{\lambda'}) \right]$$

$$= \pi \hbar \sum_{\lambda \lambda'} |I_{\lambda \lambda'}|^2 \left(-\frac{\partial f_0}{\partial E} \right)_{E_\lambda} \delta(E_\lambda - E_{\lambda'}). \tag{1.136}$$

Now we use explicitly, that $\lambda \equiv s, n, E$, and integrating over the energy E' obtain

$$G = \pi \hbar \int_{-\infty}^{\infty} \sum_{ss'} \sum_{nn'} |I_{sn,s'n'}|^2 \left(-\frac{\partial f_0}{\partial E} \right) dE$$

$$= \pi \hbar \int_{-\infty}^{\infty} \sum_{nn'} \left[|I_{Ln,Ln'}|^2 + |I_{Ln,Rn'}|^2 + |I_{Rn,Ln'}|^2 + |I_{Rn,Rn'}|^2 \right] \left(-\frac{\partial f_0}{\partial E} \right) dE. \tag{1.137}$$

The calculation of $|I_{sn,s'n'}|^2$ for the scattering states (1.113), (1.114) is straightforward, left or right parts of these expressions can be equivalently used, it is essentially the same, as we made to get (1.126). Thus, we have (here $n, n' \in L, m, m' \in R$)

$$I_{n,n'} = \frac{e}{h} \left(\hat{t}^\dagger \hat{t} \right)_{n'n}, \quad I_{n,m} = \frac{e}{h} \left(\hat{r}'^\dagger \hat{t} \right)_{n'n}, \quad I_{m,n} = -\frac{e}{h} \left(\hat{r}^\dagger \hat{t}' \right)_{nn'}, \quad I_{m,m'} = -\frac{e}{h} \left(\hat{t}'^\dagger \hat{t}' \right)_{mm'}. \tag{1.138}$$

Using this expressions and the properties (1.105), it is easy to show that in the time-reversal case

$$\sum_{ss'} \sum_{nn'} |I_{sn,s'n'}|^2 = \left(\frac{e}{h} \right)^2 \operatorname{Tr} \left[\left(\hat{t}^\dagger \hat{t} \right)^2 + \left(\hat{t}'^\dagger \hat{t}' \right)^2 + \hat{t}^\dagger \hat{r}' \hat{r}'^\dagger \hat{t} + \hat{t}'^\dagger \hat{r} \hat{r}^\dagger \hat{t}' \right] = 2 \left(\frac{e}{h} \right)^2 \operatorname{Tr} \left(\hat{t}^\dagger \hat{t} \right), \tag{1.139}$$

and finally

$$G = \frac{e^2}{h} \int_{-\infty}^{\infty} \operatorname{Tr} \left(\hat{t}^\dagger \hat{t} \right) \left(-\frac{\partial f_0}{\partial E} \right) dE. \tag{1.140}$$

We derived again the Landauer formula.

1.4 Multi-terminal systems

1.4.1 Multi-terminal Landauer-Büttiker formula

The scattering theory, developed in the previous section, can be applied also in the multi-terminal case (Fig. 1.11) exactly in the same way, as in the multi-channel case. The only difference from the considered before two-terminal system is that now there are several electrodes with independent electrochemical potentials and the same number of leads with independent transport channels.

We use in this section the following notations: M is the number of terminals, N_s ($s = 1, ..., M$) is the number of transport channels in s lead, $N = \sum_s N_s$ is the full number of channels.

The current through the terminal s, flowing in the direction to the scattering region, is given by the following expression

$$I_s = e \sum_n \left[\int_0^\infty v_s(n, k_z) f_s(n, k_z) \frac{dk_z}{2\pi} + \int_{-\infty}^0 v_s(n, k_z) \sum_{pm} |S_{sn,pm}|^2 f_p(m, k_z) \frac{dk_z}{2\pi} \right],$$

(1.141)

here s, p are the terminal indices, n, m are the channel indices. The first term is the current of the electrons incoming from the s electrode, the second term is the current of electrons reflected and transmitted from other electrodes. Changing to the energy integration, we get finally

$$I_s = \frac{e}{h} \int_{-\infty}^\infty \sum_{n, pm} \left[\delta_{sp} \delta_{nm} - |S_{sn,pm}|^2 \right] f_p(E) dE.$$

(1.142)

Let us introduce the transmission and reflection functions

$$\bar{T}_{sp} = \sum_{nm} |S_{sn,pm}|^2, \quad \bar{R}_{ss} = \sum_{nn'} |S_{sn,sn'}|^2,$$

(1.143)

by definition $\bar{T}_{ss} = \bar{R}_{ss}$. Then, the current gets the form

$$I_s = \frac{e}{h} \int_{-\infty}^\infty \left[(N_s - \bar{R}_{ss}) f_s(E) - \sum_{p \neq s} \bar{T}_{sp} f_p(E) \right] dE,$$
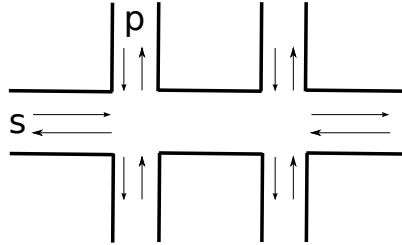
(1.144)

Fig. 1.11. Multi-terminal system.

or, equivalently,

$$I_s = \frac{e}{h} \int_{-\infty}^{\infty} \left[N_s f_s(E) - \sum_p \bar{T}_{sp} f_p(E) \right] dE, \tag{1.145}$$

or, equivalently

$$I_s = \frac{e}{h} \sum_p \int_{-\infty}^{\infty} [\bar{T}_{ps} f_s(E) - \bar{T}_{sp} f_p(E)] \, dE. \tag{1.146}$$

From the unitarity the following sum rule can be obtained

$$\sum_p \bar{T}_{sp} = \sum_p \bar{T}_{ps} = N_s. \tag{1.147}$$

From time-reversal in the presence of a magnetic field **H**

$$\sum_{p \neq s} \bar{T}_{sp}(\mathbf{H}) = \sum_{p \neq s} \bar{T}_{ps}(-\mathbf{H}). \tag{1.148}$$

1.4.2 Büttiker conductance formalism

Following Büttiker [9, 10], we formulate the elegant formulas, which allow to calculate the currents and voltages in the linear regime. We start from the current expression (1.146). For small voltages

$$G_{sp} = \frac{e^2}{h} \int_{-\infty}^{\infty} \bar{T}_{sp}(E) \left(-\frac{\partial f_0}{\partial E} \right) dE, \tag{1.149}$$

$$I_s = \sum_p [G_{ps} V_s - G_{sp} V_p]. \tag{1.150}$$

In the time-reversal case these formulas take the usual multi-channel form. For example, the formulas (1.120) and (1.121) can be rewritten as

$$I_s = \frac{e^2}{h} \sum_p \bar{T}_{sp} (V_s - V_p) = \frac{e^2}{h} \sum_{s \neq p} \bar{T}_{sp} V_{sp}, \tag{1.151}$$

$$G_{sp} = \frac{e^2}{h} \bar{T}_{sp} = \frac{e^2}{h} \text{Tr} \left(\hat{t}_{sp} \hat{t}_{sp}^\dagger \right). \tag{1.152}$$

In equilibrium $I_s = 0$, but the potentials V_s can have some constant value because of gauge invariance $V_s = V_0 \neq 0$. Thus, we obtain the sum rule

$$\sum_p G_{ps} = \sum_p G_{sp}. \tag{1.153}$$

This shows, that the current can be equivalently written as

$$I_s = \sum_p G_{sp} [V_s - V_p]. \tag{1.154}$$

There is also the alternative representation

$$I_s = \sum_p G'_{sp} V_p, \tag{1.155}$$

where the conductances $\hat{G}'$ are defined by the following $M \times M$ matrix

$$\hat{G}' = \frac{e^2}{h} [] = \frac{e^2}{h} \begin{bmatrix} N_1 - \bar{R}_{11} & -\bar{T}_{12} & \cdots & -\bar{T}_{1M} \\ -\bar{T}_{21} & N_2 - \bar{R}_{22} & \cdots & -\bar{T}_{2M} \\ \vdots & \cdots & \ddots & \vdots \\ -\bar{T}_{M1} & \cdots & \cdots & N_M - \bar{R}_{MM} \end{bmatrix}. \tag{1.156}$$

The conductances G and G' are related in an obvious way, and can be used equivalently. The sum rule for $\hat{G}'$ is

$$\sum_p G'_{ps} = 0 \;\Rightarrow\; G'_{ss} = -\sum_{p \neq s} G'_{ps}. \tag{1.157}$$

Before discussing the applications of this current formula, we should introduce the notion of a *voltage probe*. The voltage probe is any terminal, in which the zero current is preserved, $I_s = 0$. In spite of zero current, such terminal influences the current through other terminals. The physical reason is that the electrons can enter the electrode and return back, but after phase randomization. Thus, the voltage probe can be used not only for voltage measurement, but also for introducing a decoherence into the system.

3-terminal conductance

Consider as an example, a three-terminal junction (Fig. 1.12). Let us consider the terminal 3 as a voltage probe: $I_3 = 0$, $I_1 = -I_2 = I$, $V_1 - V_2 = V$. We have the following equations

$$I_3 = G_{31}(V_3 - V_1) + G_{32}(V_3 - V_2) = 0, \tag{1.158}$$

$$I = G_{12}V + G_{13}(V_1 - V_3) = G_{21}V - G_{23}(V_2 - V_3). \tag{1.159}$$

We can also choose $V_1 = V$, $V_2 = 0$, then

$$V_3 = \frac{G_{31}}{G_{31} + G_{32}} V. \tag{1.160}$$

This voltage is not small in the limit $G_{31}, G_{32} \ll G_{12}$, when the third electrode is used for unperturbed voltage measurement. The current is

$$I = \left[G_{12} + \frac{G_{13}G_{32}}{G_{31} + G_{32}} \right] V, \tag{1.161}$$

it is not perturbed when $G_{31}, G_{32} \to 0$, but at finite coupling to the third electrode, the current between electrodes 1 and 2 is changed.

4-terminal conductance

Consider now the 4-terminal system (Fig. 1.12) and assume that electrodes 3 and 4 are weakly coupled voltage probes. Ih this case the current $I = I_1 = -I_2 \approx G_{12}V$. What is the voltage $V' = V_3 - V_4$? Neglecting G_{34} and G_{43} as the next-order small terms, we obtain

$$V' = \frac{G_{31} - G_{32}}{G_{31} + G_{32}}V \approx RT,\tag{1.162}$$

and

$$G = \frac{I}{V'} = \frac{e^2}{h}\frac{R}{T}.\tag{1.163}$$

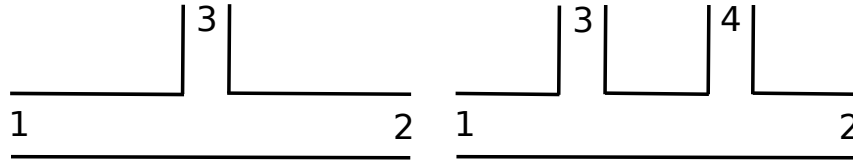We obtained the first Landauer formula.

Fig. 1.12. 3 and 4 terminal junctions.

1.4.3 Edge states in quantum Hall effect

Problems

1.1 Inter-mode scattering in an adiabatic waveguide

Find the nonadiabatic corrections Δ_n to the equation (1.7)

$$\left\{ -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial z^2} + E_n(z) \right\} \psi_{nE}(z) = E\,\psi_{nE}(z) + \Delta_n. \qquad (1.164)$$

1.2 Transmission though a symmetric rectangular barrier

Consider the rectangular barrier

$$U(z) = \begin{cases} 0, & z < -a, \\ U_0, & -a < z < a, \\ 0, & z > a. \end{cases} \qquad (1.165)$$

The wave function is given by

$$\psi(z) = \begin{cases} A_+ e^{ikz} + A_- e^{-ikz}, & z < -a \\ C_1 e^{-\kappa z} + C_2 e^{\kappa z}, & -a < z < a \\ B_- e^{ikz} + B_+ e^{-ikz}, & z > a \end{cases} \qquad (1.166)$$

where

$$k = \frac{\sqrt{2mE_z}}{\hbar}, \qquad (1.167)$$

$$\kappa = \frac{\sqrt{2m(U_0 - E_z)}}{\hbar}. \qquad (1.168)$$

Show that

$$T(E_z < U_0) = \frac{4k^2\kappa^2}{(k^2 + \kappa^2)^2 \sinh^2(a\kappa) + 4k^2\kappa^2}, \qquad (1.169)$$

$$T(E_z > U_0) = \frac{4k^2\kappa^2}{(k^2 - \kappa^2)^2 \sin^2(a\kappa) + 4k^2\kappa^2}. \qquad (1.170)$$

1.3 Transmission though a δ-barrier with asymmetric leads

1.4 Transmission though an asymmetric rectangular barrier

Other problems